Phase transition in exotic nuclei along the $N = Z$ line

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The abrupt structure change from the nuclei of $N = Z \leq 35$ to those of $N = Z \geq 36$ is investigated by means of shell model calculations. The basic features of the even-even and odd-odd nuclei under consideration are nicely reproduced. A sudden jump of nucleons into the upper $g_{9/2}d_{5/2}$ shell at $N = Z = 36$ is found to be the main reason that causes the qualitative structure difference. It is argued that the structure change can be viewed as a decisive change of the mean field, or a phase transition, along the $N = Z$ line.

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Phase transition in a many-body system refers to an abrupt, qualitative change in wave function or mean field. This subject is of common interest for many subfields. Nuclei, being finite quantum systems composed of strongly correlated protons and neutrons, uniquely display transitional features. Often discussed in nuclei are two types of phase transition: the phase transition to superfluidity and to deformation. The first one is easy to trace with the standard BCS theory which gives the critical condition [1]. The second one, the transition to deformation, takes place as some control parameters vary along an isotopic (isotonic) chain, which, for example, brings the system from a spherical to a deformed region.

The second type of phase transition, also called shape phase transition [2], has been theoretically studied but mainly by means of algebraic models [3]. Well-suited cases are those described by an algebraic Hamiltonian with a dynamical group, where a transition-driving control parameter appears explicitly in the Hamiltonian. Large-scale shell model descriptions [4, 5] for deformation in medium-mass nuclei have become possible in recent years. The shell model can provide a more fundamental basis to the study of shape phase transition. In fact, the Monte Carlo Shell Model calculation [6] has shown the first example. The advantage of a shell model study is that one may see microscopically the origin of a phase transition by analyzing the wave functions if transition-driving mechanism is contained in the effective interaction. The aim of the present Letter is to carry out such a study using the spherical shell model, to show a shape phase transition in $A \sim 70$ nuclei along the $N = Z$ line, and to understand the cause of the transition by studying the occupations in the nucleon orbits.

The $N = Z$ nuclei around $A \sim 70$ exhibit several unique phenomena [7, 8], and therefore have attracted many theoretical and experimental studies. This is possibly due to the rather strong proton-neutron correlations in these nuclei since protons and neutrons occupy the same orbits. In particular, there is apparently an abrupt change in structure when the proton and neutron numbers cross $N = Z = 35$, which can be clearly seen from the graph of spin J versus angular frequency $\omega = (E(J) - E(J-2))/2$ (the so-called $J - \omega$ graph). Fig. 1 shows a separation of two groups for the $N = Z$ nuclei from ^{64}Ge to ^{76}Sr, one with larger ω's corresponding to smaller moments of inertia and another with smaller ω's corresponding to larger moments of inertia. In the left group, ^{76}Sr takes a straight line whose extension intersects the origin of the $J - \omega$ graph. Thus ^{76}Sr behaves like a rotor with a large and approximately constant moment of inertia J/ω. The $J - \omega$ curves for ^{72}Kr and ^{74}Rb show that these nuclei have a structure rather similar to that of ^{76}Sr although the lowest state of ^{72}Kr appears to be peculiar (see discussions below). In contrast, the nuclei in the right group with $N = Z \leq 35$, which resemble each other, have a moment of inertia only approximately half of the values of the left group. This sharp difference suggests a qualitative structure change between the nuclei with $N = Z \leq 35$ and $N = Z \geq 36$. No nuclei sit in between, implying that the structure change with nucleon number is sudden.

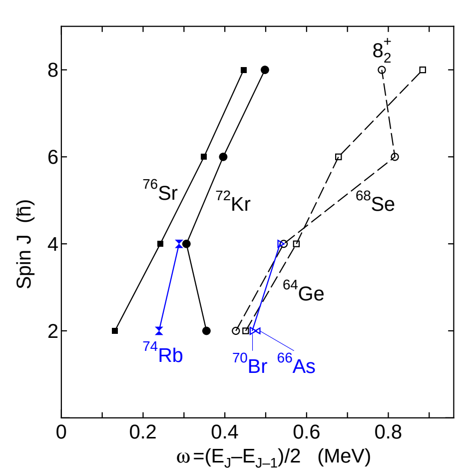

FIG. 1: (Color online) The known experimental data shown in the graph of spin J versus angular frequency ω.

The above structure change along the $N = Z$ line may be comparable to that near $N = 40$ in Ge isotopes [9], which has been observed in the (p,t) cross sections and $B(E2; 0_1^+ \to 2_1^+)$ values. For example, ^{72}Ge has an unusually low second 0^+ state below the 2_1^+ state, and so does ^{72}Kr [10]. In a separate study for Ge isotopes [11], we have discovered the possible sources for the structure change near $N = 40$. The study suggests that the change is caused mainly by a sudden jump of nucleons into the $g_{9/2}$ orbit. We may expect that the $g_{9/2}$ occupation is also the leading source for the structure change along the $N = Z$ line.

In the early study [11], we found it difficult to get a sufficient $g_{9/2}$ contribution within the $pf_{5/2}g_{9/2}$ shell model, in spite of the fact that this model space is capable of describing the nuclei ^{64}Ge and ^{68}Se [12]. On the other hand, the Shell Model Monte Carlo calculations [13] suggest that the $d_{5/2}$ orbit has a cooperative effect that enhances the $g_{9/2}$ contribution. Thus the $pf_{5/2}g_{9/2}d_{5/2}$ shell model can be a hopeful model to investigate the structure change shown in Fig. 1. This model space is, unfortunately, too large to perform a shell model calculation. The model space that we can presently handle is a truncated one $f_{5/2}p_{1/2}g_{9/2}d_{5/2}$. (Note that calculation for ^{76}Sr can be performed by using the extrapolation method [14].) Setting nucleons in the $p_{3/2}$ orbit inactive is a severe restriction since correlations in the fp shell are strong. Nevertheless, this can be compromised by adjusting effective interactions. The choice of the present model space seems to have grasped the basic physics, as we discuss below.

With the extended $P + QQ$ Hamiltonian [11, 12], we have searched for suitable parameters that can reproduce the experimental data in this mass region. The level schemes shown in Fig. 2 are obtained by using the following set of parameters. Single-particle energies for the $f_{5/2}$, $p_{1/2}$, $g_{9/2}$, and $d_{5/2}$ orbits are 0.0, 0.3, 1.5 and 2.0 MeV, respectively. For interaction strengths, we take

$$g_0 = 0.25(68/A), \quad g_2 = 0.16(68/A)^{5/3},$$
$$\chi_2 = 0.14(68/A)^{5/3}, \chi_3 = 0.04(68/A)^2 \text{ in MeV.} \quad (1)$$

The average $T = 0$ monopole field and $T = 1$ monopole corrections (in MeV) are fixed as follows:

$$k^0 = H_{\rm mc}^{T=0}(a,b) = -0.63(68/A) \text{ for arbitrary } (a,b),$$
$$H_{\rm mc}^{T=1}(f_{5/2}, p_{1/2}) = -0.6,$$
$$H_{\rm mc}^{T=1}(f_{5/2}, g_{9/2}) = H_{\rm mc}^{T=1}(f_{5/2}, d_{5/2}) = -0.5,$$
$$H_{\rm mc}^{T=1}(g_{9/2}, g_{9/2}) = 0.2, H_{\rm mc}^{T=1}(d_{5/2}, d_{5/2}) = -0.18. \quad (2)$$

It is found that to excite nucleons more efficiently to the upper orbits $(g_{9/2}, d_{5/2})$, we should take a small $d_{5/2}$ single-particle energy close to the $g_{9/2}$ one and large monopole corrections $H_{\rm mc}^{T=1}(f_{5/2}, g_{9/2})$ and $H_{\rm mc}^{T=1}(f_{5/2}, d_{5/2})$. The above parameter set may be named "the effective interaction of the small model".

Calculated level schemes for the $N = Z$ nuclei ^{68}Se, ^{72}Kr, ^{76}Sr, and the $N = Z+2$ nucleus ^{74}Kr are compared with experimental data in Fig. 2. Both the ground band (in black) and the first excited 0^+ band (in blue) are shown for each nucleus. The truncated space without the $p_{3/2}$ orbit cannot perfectly reproduce the data. However, the qualitative feature for each nucleus is well described. The ^{68}Se nucleus is seen to have a different structure with much larger energy intervals than the other three nuclei. What we find remarkable is that the calculation correctly gives the first excited 0_2^+ state in ^{72}Kr below the 2_1^+ one, in agreement with the experimental finding [10].

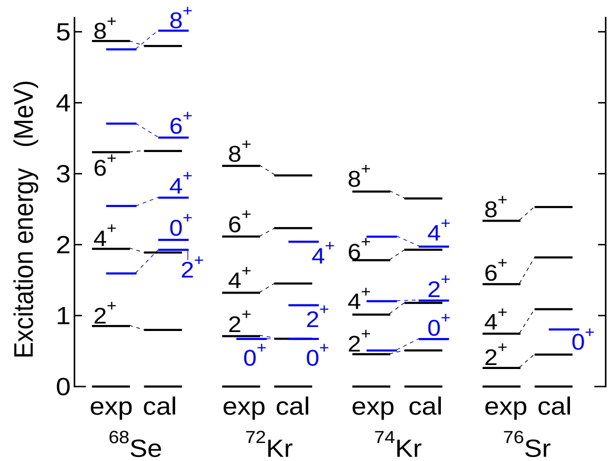

FIG. 2: (Color online) Comparison of experimental and calculated level schemes for ^{68}Se, ^{72}Kr, ^{74}Kr, and ^{76}Sr.

To trace the microscopic origin of the structure changes, we calculate nucleon occupation numbers $\langle n_a \rangle$ in respective orbits. As we employ the isospin invariant Hamiltonian, the proton and neutron occupation numbers in $N = Z$ nuclei are equal to each other, *i.e.,* $\langle n_a^\pi \rangle = \langle n_a^\nu \rangle$. To simplify the notation, we abbreviate the lower orbits $(f_{5/2}, p_{1/2})$ and the upper orbits $(g_{9/2}, d_{5/2})$ to "fp" shell and "gd" shell, respectively. We suppose that the former represents the fp shell and the latter the gd shell.

The calculated occupation numbers are shown in Fig. 3. As seen in Fig. 3a, nucleons in ^{68}Se have a negligible occupation in the "gd" shell. Although the 0_2^+ state has a different configuration from the states of the ground band, all of the states are basically constructed in the "fp" shell. We should mention that the description for ^{68}Se with the present model space may be too simplified. However, a more realistic calculation for ^{68}Se in the $pf_{5/2}g_{9/2}$ shell (including the $p_{3/2}$ orbit) [12] does not give a structure much different from the present one. We have confirmed this by improving the $pf_{5/2}g_{9/2}$ shell model so as to reproduce well the observed coexisting oblate and prolate bands [15]. We thus conclude with confidence that the ^{68}Se nucleus does not essentially occupy the "gd" shell.

In contrast to ^{68}Se, approximately two protons and two neutrons jump into the "gd" shell in the ground state 0_1^+ and the first excited state 2_1^+ in ^{76}Sr (see Fig. 3c).

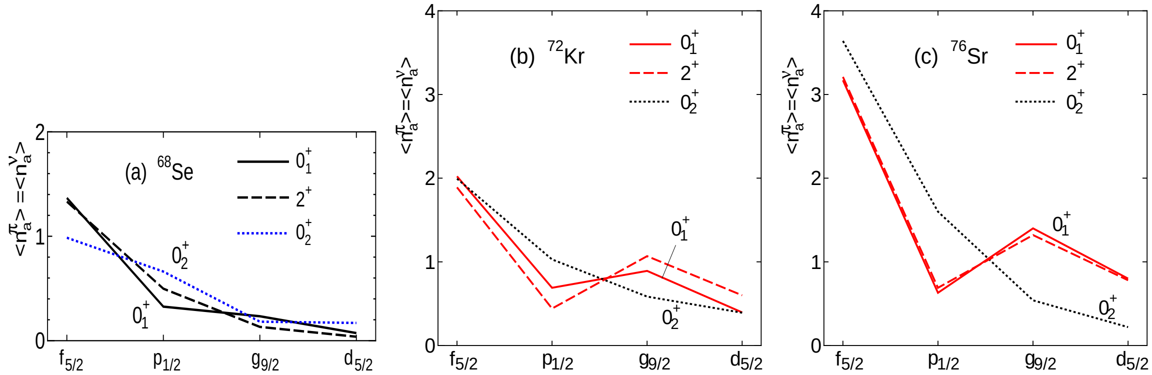

FIG. 3: (Color online) Proton and neutron occupation numbers in ^{68}Se, ^{72}Kr, and ^{76}Sr.

Similarly, nucleons in ^{72}Kr also start to occupy the "gd" shell (see Fig. 3b). These results indicate that for ^{76}Sr and ^{72}Kr, the 0_2^+ state instead of the ground state has the ordinary type of configuration, *i.e.,* the occupation number deceases gradually as the single-particle energy increases. The ground state has the dominant configuration $(\text{“}fp\text{”})^{n-4}(\text{“}gd\text{”})^4$, the probability of which is about 0.45 in ^{72}Kr and is more than 0.7 in ^{76}Sr.

The wave functions of the 0_1^+ and 0_2^+ states in ^{72}Kr have the following weights for the leading configurations:

$$
\begin{aligned}
|0_1^+\rangle &: 0.22(\text{“}fp\text{”})^8 + 0.45(\text{“}fp\text{”})^4(\text{“}gd\text{”})^4 + \cdots, \\
|0_2^+\rangle &: 0.47(\text{“}fp\text{”})^8 + 0.40(\text{“}fp\text{”})^4(\text{“}gd\text{”})^4 + \cdots. \quad (3)
\end{aligned}
$$

These numbers show that the ground state is constructed starting from the excited configuration $(\text{“}fp\text{”})^4(\text{“}gd\text{”})^4$ and the second 0^+ state is constructed starting from $(\text{“}fp\text{”})^8$. The two 0^+ states must reverse their order in energy if interactions were increased gradually in a treatment of the perturbation theory. This reversal manifests itself in the occupation numbers in Fig. 3b; the 0_1^+ state has less nucleons in the "fp" shell and more nucleons in the "gd" shell as compared to the 0_2^+ state. As shown in Fig. 3c, ^{76}Sr has the same characteristic occupation numbers obtained with the extrapolation method.

The calculation thus reveals a large difference in occupation numbers between ^{68}Se and ^{72}Kr, which correlates with their qualitatively different picture in the $J-\omega$ graph in Fig. 1. It has been known that states corresponding to both oblate and prolate shapes coexist in ^{68}Se [15]. Now our result that the ground state is constructed mainly in the fp shell suggests that the mean field of ^{68}Se is deformed but does not lie very far from the spherical one of shell model. In contrast, the ^{72}Kr ground state cannot be described in the perturbation theory based on the "fp" configuration. This means that a decisive, sudden breaking of the spherical mean field of shell model occurs when going from ^{68}Se to ^{72}Kr. We may call the abrupt change in mean field "phase transition". Then what mean field is formed after the breaking of the spherical shell model one? The occupation of the "gd" shell in ^{72}Kr and ^{76}Sr implies a definite formation of the Nilsson orbits in the deformed mean field. The transition to ^{72}Kr must be a shape phase transition. In fact, the level scheme of ^{76}Sr shows a rigid rotor behavior as seen in Fig. 1, which is qualitatively different from the nuclei with $N = Z \leq 35$. It has been discussed with the deformed mean field language [7, 16] that there is a rapid change in deformation with the deformation parameter β from ~ 0.25 in ^{68}Se, ~ 0.4 in ^{72}Kr, and ~ 0.5 in ^{76}Sr. The $g_{9/2}$ orbit has been considered to drive deformation in this mass region [17].

It has been found that in ^{72}Kr, the nearby 0_1^+ and 0_2^+ states coexist with different shapes; the excited one is considered as a shape isomer [10, 18]. In our wave functions (3), the 0_2^+ state has a very large component of the $(\text{“}fp\text{”})^4(\text{“}gd\text{”})^4$ configuration which is the main component of the 0_1^+ state, while the 0_1^+ state has a large component of the $(\text{“}fp\text{”})^8$ configuration which is the main component of the 0_2^+ state. The situation that these two 0^+ states mutually have both configurations with considerable amount in the wave functions suggests a rather strong coupling between the two states. Such a strong coupling can explain why the moment of inertia of the 2_1^+ state in ^{72}Kr deviates from the regular rotor behavior (see Fig. 1); it is simply because the 0_1^+ energy is pushed down by the coupling.

To test the model's reliability, we should also calculate the odd-odd nuclei ^{70}Br and ^{74}Rb. Calculated energy levels are compared with experimental data [19, 20] in Fig. 4. The agreement between calculation and experiment is satisfactory for the restricted model. It is found that the configuration $(\text{“}fp\text{”})^6$ is dominant in the ground state of ^{70}Br. Contrary to this, for ^{74}Rb the configuration $(\text{“}fp\text{”})^6(\text{“}gd\text{”})^4$ is leading in the low-lying collective states in the $T = 1$ band (0^+,2^+,4^+) and $T = 0$ band (3^+,5^+,7^+). These results are consistent with the clear difference in their moments of inertia between ^{70}Br and ^{74}Rb (Fig. 1). We thus reach the same conclusion that the structure of ^{74}Rb is qualitatively different from that of ^{70}Br and a shape phase transition takes place at $Z = N = 35$.

The structure change along the Ge isotopic chain manifests itself also in a rapid increase of $B(E2; 0_1^+ \to 2_1^+)$

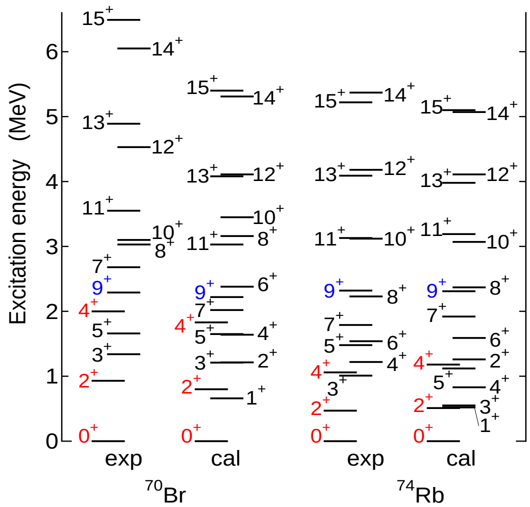

FIG. 4: (Color online) Experimental and calculated level schemes for ^{70}Br and ^{74}Rb.

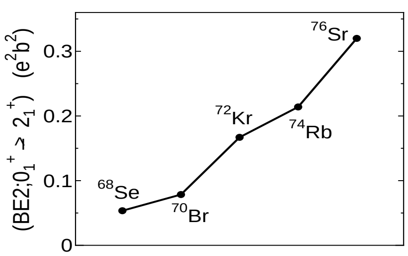

FIG. 5: Calculated $B(E2)\uparrow$ values for $A = 68 - 76$ nuclei.

[11]. Similar increase of $B(E2)\uparrow$ is expected when N exceeds 35 along the $N = Z$ line. In Fig. 5 the calculated $B(E2)\uparrow$ values from ^{68}Se to ^{76}Sr clearly show such a feature. Here, we used the effective charges $e_\pi = 1.5e$ and $e_\nu = 0.5e$. From the above analysis, the rapid increase in $B(E2)\uparrow$ is attributed to the fact that more degrees of freedom are opened up for the quadrupole correlation as nucleons occupy the "gd" shell. Thus the present results support our previous prediction [11] that the notable increase of $B(E2)\uparrow$ at $N = 40$ in Ge isotopes is caused by a jump of nucleons into the "gd" shell.

We note that our truncated model space exposes its weakness in reproduction of absolute value of $B(E2)\uparrow$. For ^{72}Kr, the calculated value 0.17 e^2b^2 is only about one third of the observed one ~ 0.5 e^2b^2 [17]. However, we know the possible reason for the discrepancy. The shell model for ^{68}Se with the $pf_{5/2}g_{9/2}$ space [12] gave the $B(E2)\uparrow$ value 0.16 e^2b^2, which is about three times as large as the present result 0.054 e^2b^2. Including the $p_{3/2}$ orbit, which contributes to correlations in the fp shell, will enhance the $B(E2)\uparrow$ values considerably. For ^{68}Se, while the $pf_{5/2}g_{9/2}$ shell model [12] reproduced a positive spectroscopic quadrupole moment (Q_{sp}) corresponding to an oblate shape for the 2_1^+ state, the present model fails. This suggests that the lack of the $p_{3/2}$ orbit is a serious problem for those quantities sensitive to the details of wave functions. Obviously it requires a larger model space to describe these quantities.

In conclusion, the experimental level schemes of the $A \sim 70$ $N = Z$ nuclei show clearly an abrupt structure change at $N = Z = 36$. We have investigated this problem by means of large-scale shell model calculations. In spite of the limit of the practicable model space, we have been able to reproduce the basic features of the level schemes. Through analyzing the wave functions, we have concluded that the qualitative structure difference between the nuclei with $N = Z \leq 35$ and those with $N = Z \geq 36$ has the origin of the upper "gd" shell occupation. It has been discussed that the structure change is caused by a decisive breaking of the spherical shell model mean field and a formation of deformed mean field. In this sense, we have witnessed a basic mechanism of the phase transition to deformation in nuclei. We note that calculations in a space larger than $pf_{5/2}g_{9/2}d_{5/2}$ must be carried out to describe deformation properly.

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